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Doping O into Conventional GeTe/Sb_2Te_3 Superlattice for Functional Material of Artificial Synapse

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Abstract. Brain-like systems potentially with extremely low power consumption and fast speed, are composed of artificial neurons and synapses. In this study, we adopted GeTe/Sb_2Te_3 superlattice as the synaptic functional base materials due to its low power consumption and ns-order fast speed. In the conventional GeTe/Sb_2Te_3 superlattice device, the synaptic strength is changed via Ge atom transfer but only two states are obtained in many cases. In this work, in order to enable multi-state changes required for most practical artificial synapses, we investigated the influence of doping O into the GeTe/Sb_2Te_3 superlattice on the band structure for a wide bandgap based on first-principles study.

1. Introduction

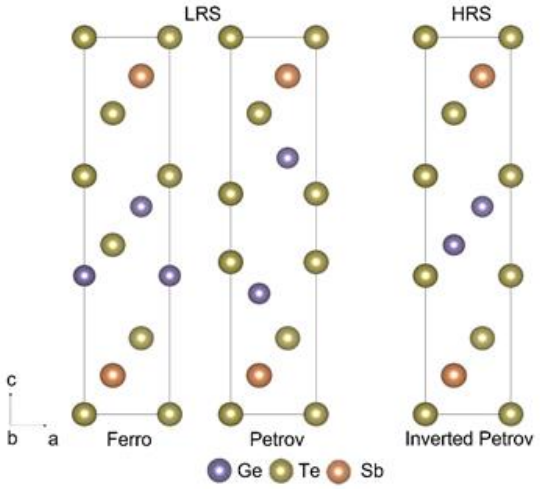
Neuromorphic computing has gained significant attention globally due to its potential to overcome the von Neumann bottleneck and efficiently handle tasks like pattern recognition, fuzzy logic, and associative learning [1]. Besides commonly used oxides [2, 3], chalcogenides like $Ge_2Sb_2Te_5$, known for their amorphous-crystalline phase transition in the order of 10 ns, have been utilized to mimic synaptic functions for achieving neuromorphic computing [4]. Additionally, the phase-change memory employing a chalcogenide-based superlattice structure such as GeTe/Sb_2Te_3 has shown promise by demonstrating substantial resistance changes without the conventional phase transition seen in $Ge_2Sb_2Te_5$, resulting in a considerable reduction in power consumption [5]. The GeTe/Sb_2Te_3 superlattice, particularly the application to artificial synapses, has been explored recently. However, achieving the intermediate states crucial for synaptic plasticity has been challenging [6]. In this study, attempts were made to incorporate oxygen (O) into GeTe/Sb_2Te_3 superlattice to widen the bandgap. The O doping of effect on the band structure was here investigated by first-principles study.

2. Simulation method and model

Atomic and electronic structures were obtained using Advance/PHASE, a commercial software for first-principles calculations based on density functional theory with plane-wave basis and pseudopotentials. For structure optimization, k points were sampled on a 3*3*3 mesh. The cutoff energy of the plane-wave basis was set to 272.1 eV. Xgdiis method was used for structure optimization, in which all atoms were relaxed until the force was smaller than 0.0272 eV. Spin-polarization and spin-orbit interaction were not included in the calculations.

To artificially form a layered structure, hexagonal crystals are easy to stack. There are no other arrangements in which the Te atomic layer and Ge layer face each other except I-(Ge-Te-Ge-Te), II-(Ge-Te Te-Ge), and III-(Te-Ge Ge-Te). In this study, referring to the speculation from previous studies that a larger distance of Ge results in a larger bandgap, II-(Ge-Te Te-Ge) and III-(Te-Ge Ge-Te) were

employed to analyze the high and low resistivity bandgaps [7]. Fig.1 shows atomic structure of Inverted



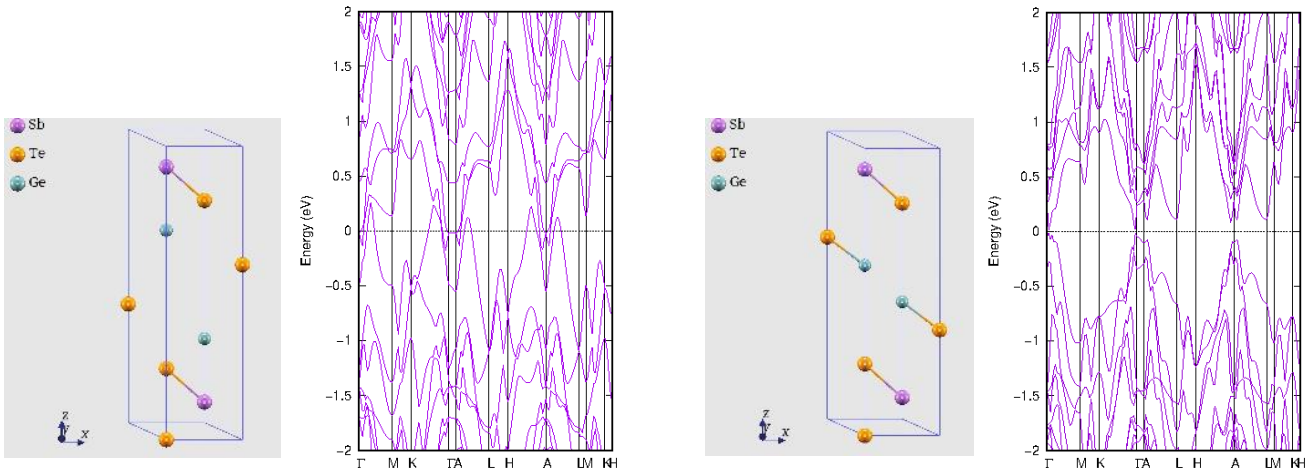
Petrov structure (HRS), Ferro structure and Petrov structure (LRS).

Fig.1 Atomic structure of Inverted Petrov structure (HRS), Ferro structure and Petrov structure (LRS)

3. Results and discussion

3.1 $GeTe/Sb_2Te_3$ superlattice phase-change method

Figures 2(a) and 2(c) show the Petrov and Inverted Petrov structures of a conventional undoped $GeTe/Sb_2Te_3$ superlattice primitive cell consisting of atomic layers of -Te-Sb-Te-Ge-Te-Te-Ge-Te-Sb-Te- and -Te-Sb-Te-Te-Ge-Ge-Te-Te-Sb-Te-, respectively. Figures 2(b) and 2(d) show the corresponding band structures of the two superlattice structures. Figure 3 shows that the Petrov structure is metallic and in a low-resistivity state (LRS), while the Inverted Petrov structure is semiconducting and in a high-resistivity state (HRS). In the HRS, the bandgap is indicated as 0.22 eV. The switching between the high- and low-resistivity states can be achieved by a slight structural change based on the migration of Ge and Te atoms, rather than the conventional amorphous-crystalline phase transition.



(a) (b) (c) (d)

Fig. 2 (a) Atomic structure and (b) band structure of Petrov structure, (c) atomic structure and (d) band structure of Inverted Petrov structure of undoped superlattice $GeTe/Sb_2Te_3$.

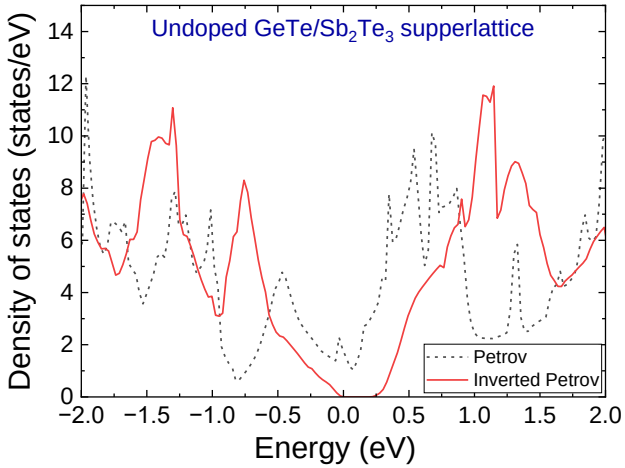
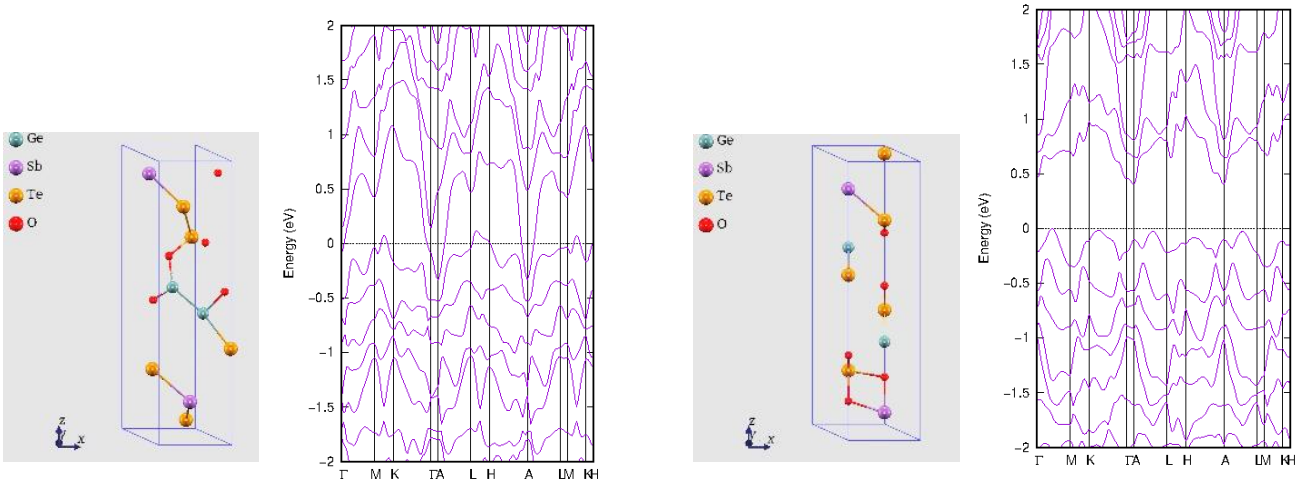


Fig. 3 Density of states of Petrov structure and Inverted Petrov structure of undoped superlattice $GeTe/Sb_2Te_3$.

3.2 O-doped $GeTe/Sb_2Te_3$

Figures 4(a) and 4(c) show Petrov and Inverted Petrov structures for an O-doped $GeTe/Sb_2Te_3$ superlattice primitive cell with five O atoms incorporated. The structural optimization results show that the atomic structure after doping with a large amount of O is quite different from that of the undoped superlattice. Figures 4(b) and 4(d) show the corresponding band structures of the two superlattice structures. It is clear from Figure 5 that the bandgap after doping is about twice wider than that of the conventional Petrov superlattice. For the O-doped Inverted Petrov superlattice, the bandgap is shown to be 0.44 eV. This suggests that doping O into conventional $GeTe/Sb_2Te_3$ superlattices can control the resistance (or conductance, synaptic weight) for the application to artificial synapses.



(a) (b) (c) (d)

Fig. 4 (a) Atomic structure and (b) band structure of Petrov structure, (c) atomic structure and (d) band structure of Inverted Petrov structure of O-doped superlattice $GeTe/Sb_2Te_3$.

4. Conclusion

Based on our simulation results, we can draw the following conclusions.

(1) In $GeTe/Sb_2Te_3$ superlattice structure, no conventional amorphous-crystalline transition is necessary for the resistance switching because the resistance was caused by changing the bonding state of Ge and Sb.

(2) Doping O into conventional $GeTe/Sb_2Te_3$ superlattice enables us to control the bandgap. This implies that the performance the artificial synapse can be well improved.

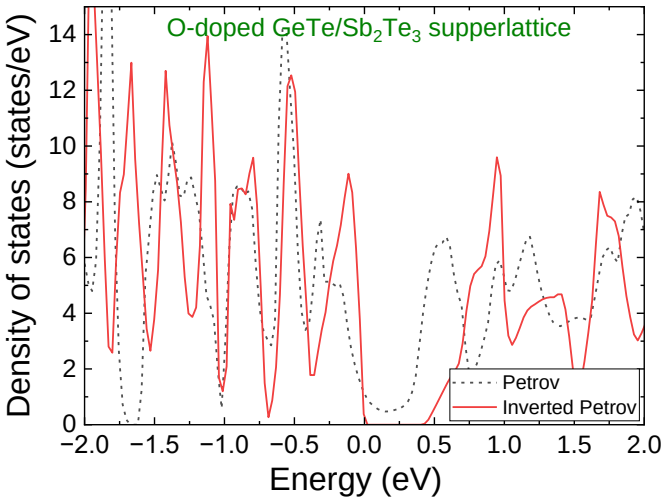


Fig. 5 Density of states of Petrov structure and Inverted Petrov structure of O-doped superlattice $GeTe/Sb_2Te_3$.

Acknowledgements

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